RESEARCH HIGHLIGHTS
Basic Energy Sciences Program
Geosciences Subprogram

Title: Lattice-Gas Modeling of Retardation and Buoyancy in Fractures

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Objective: To test the effects of buoyancy and scaling on the extrapolation of dispersion and retardation coefficients from lab to field scale.

Results: The lattice-gas automata and lattice Boltzmann (BGK) methods were used to estimate the mixing of fluid streams at a continuous fracture junction, for Peclet number $\boldsymbol{Pe}$ from 0 to 1547. Agreement with experimental results is good, particularly at $\boldsymbol{Pe} \leq 25$. At low $\boldsymbol{Pe}$, a large fracture length/width is needed to obtain accurate mixing ratios ($\boldsymbol{M_r}$). For a 90° intersection of two fractures with equal widths and flow rates, $\boldsymbol{M_r}$ approaches 0.5 (complete mixing) at $\boldsymbol{Pe} \approx 1$. At the highest $\boldsymbol{Pe}$ studied, $\boldsymbol{M_r} = 0.022$, in contrast with the streamline routing prediction $\boldsymbol{M_r} = 0$.

Significance: Discrete fracture network models are used to predict the fate and transport of contaminants. Fractured environments of interest to DOE include Yucca Mountain, and the basalts at Hanford and INEEL. However, the intense scrutiny afforded fracture network models at the British Selafield site has left doubts about the validity of this approach (see, for example, `http://www.foe.co.uk/nirexrcf/foe6.html`). Commercial applications of these models include oil and gas production, and the prediction of organic contaminant migration. For example, the transport of DNAPLS to the accessible environment usually involves two steps; an initial, rapid sinking into fractured rock or sediments; and the dissolution and dispersion of the DNAPLS in ground water and subsurface air. The latter is the real mechanism of transport and exposure to humans, and under remediation conditions, can occur at high $\boldsymbol{Pe}$.

Fracture network models must apply a mixing rule at fracture intersections, to account for the splitting and redistribution of solute in the fluid streams; without a rigorous mixing rule, it is hard to place confidence in network models as predictive tools. There are two popular mixing algorithms: complete mixing (for $\boldsymbol{Pe} = 0$) and streamline routing (for $\boldsymbol{Pe} = \infty$). The behavior at intermediate $\boldsymbol{Pe}$ is critical to network modeling; however, prior to our work, the only available numerical analysis of junction mixing gave highly controversial results, suggesting that very little mixing occurred, even at very low $\boldsymbol{Pe}$ (these results were at odds with lab experiments conducted by Chunhong Li). We used LGA and LB methods to calculate mixing as a function of $\boldsymbol{Pe}$ number, obtained good agreement with lab experiments, and showed why previous numerical methods gave contradictory results.

Publication: Stockman, H.W.; Li, C. and Wilson, J.L. (1997) A lattice-gas and lattice Boltzmann study of mixing at continuous fracture junctions: Importance of boundary conditions, accepted for ***Geophysical Research Letters***.

Figure: The fracture mixing problem; geometry at left, and comparison of LB and LGA with experiments and previous numerical analysis at right.